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Vapor Pressures and Boiling Points of Sixty API-NBS Hydrocarbons[1]

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Measurements of vapor pressures and boiling points, over the range 48 to 780 millimeters of mercury, and above about 11° C, were made on 60 purified hydrocarbons. The apparatus consisted of an electrically heated boiler, a vapor space with a vertical reentrant tube containing a platinum thermometer having a resistance of 25 ohms, and a condenser. Measurements of the temperature of the liquid-vapor equilibrium were made at 20 fixed pressures maintained automatically. The values of the fixed pressures were determined by calibration of the apparatus with water using the vapor pressure-temperature tables prepared at this Bureau.

The experimental data on the hydrocarbons were correlated, the method of least squares being used, with the three-constant Antoine equation for vapor pressures, log $P=A-B/(C+t)$ or $t=B/(A-\log P)-C$. Experimental data, together with the values of the three constants of the Antoine equation applicable over the range of measurement, are reported for 60 API–NBS hydrocarbons, including 17 paraffins, 14 alkylcyclopentanes, 8 alkylcyclohexanes, and 21 alkylbenzenes.

I. Introduction

This investigation is part of the systematic program of determining physical properties of highly purified hydrocarbons being prepared in the cooperative program of the American Petroleum Institute and the National Bureau of Standards. Measurements of vapor pressures and boiling points were made over the range 48 to 780 mm Hg, and above about 11° C, on 60 hydrocarbons of the API-NBS series. This paper gives the experimental data, and results of the correlation with the Antoine equation, for 17 paraffin, 14 alkylcyclopentane, 8 alkylcyclohexane, and 21 alkylbenzene hydrocarbons.

II. Apparatus and Procedure

The apparatus and procedure employed in this investigation were essentially similar to those already described [1].[3] The modifications consisted of increasing the thermometric sensitivity from 1.4 to 3.3 mm of scale deflection per 0.001° C; installing a new condenser and reflux regulator patterned after one previously described [2]; blending the heat of a reentrant 50-watt heater with that of the external heater, wrapped around the boiler, to minimize bumping at low pressures; and connecting a high-pressure nitrogen cylinder, with suitable reducing values and drying train, to the inlet of the ballast tank. The nitrogen cylinder obviated the use of a pressure pump for measurements above 1 atmosphere and permitted boiling without contact with oxygen.

III. Determination of Pressures

The values of the pressures produced by the apparatus, when controlled at the 20 fixed contacts, were determined from periodic measurements of the temperature of the liquid-vapor equilibrium made with water in the apparatus. The changes in these values were substantially the same as those previously reported [1]. The vapor pressure of water at 1-deg. intervals from 35° to 103° C was taken from table 2 of Osborne and Meyers [3], together with unpublished small revisions of

[1] This investigation was performed at the National Bureau of Standards as part of the work of the American Petroleum Institute Research Project 6 on the "Analysis, Purification, and Properties of Hydrocarbons."

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[3] Figures in brackets indicate the literature references at the end of this paper.

these values by Meyers, Stimson, and Cragoe [4]. From these values, several values were interpolated (by Lagrangian five point curvilinear interpolation) at 0.1-deg. intervals in the neighborhood of the temperature of the liquid-vapor equilibrium for water at each of the 20 fixed pressures. The final calculation of the pressure at each observed temperature was made by linear interpolation within the 0.1-deg. intervals.

IV. Source and Purity of Compounds

The compounds whose vapor pressures were measured in the present investigation were samples from the API–NBS series of highly purified hydrocarbons, which are being prepared through a cooperative undertaking of the American Petroleum Institute and the National Bureau of Standards. The description of the compounds is given in a preceding report [5], with the purification and determination of purity and freezing points of these compounds described in references [6, 7, 8, 9, 10]. It is believed that in each case the impurity was of such nature and present in such small amounts that the properties measured were not affected beyond the indicated limits of uncertainty.

V. Experimental Data on 60 API–NBS Hydrocarbons

In table 1 are given the experimental data on the temperatures and pressures of the liquid-vapor equilibrium for 17 paraffin, 14 alkylcyclopentane, 8 alkylcyclohexane, and 21 alkylbenzene hydrocarbons.

TABLE 1. *Experimental data for 60 hydrocarbons on the temperatures and pressures of the liquid-vapor equilibrium*

t	P	t	P	t	P	t	P	t	P
n-Heptane		2-Methylhexane		3-Methylhexane		3-Ethylpentane		2,2-Dimethylpentane	
°C	*mm* Hg	°C	*mm* Hg	°C	*mm* Hg	°C	*mm* Hg	°C	*mm* Hg
99.322	780.20	90.936	780.13	92.737	780.13	94.367	780.12	---------	---------
98.813	768.63	90.430	768.58	92.229	768.58	93.856	768.58	80.074	780.13
98.237	755.75	89.860	755.62	91.655	755.61	93.277	755.61	79.573	768.58
97.728	744.49	89.357	744.40	91.148	744.40	92.771	744.39	79.005	755.61
97.180	732.53	88.814	732.46	90.602	732.46	92.238	732.46	78.508	744.39
92.078	628.32	83.769	628.24	85.529	628.24	87.119	628.23	77.970	732.46
84.856	501.15	76.628	501.07	78.347	501.07	---------	---------	72.968	628.23
78.202	402.93	70.051	402.84	71.732	402.84	73.242	402.84	65.895	501.07
71.966	325.42	63.889	325.31	65.533	325.41	---------	---------	59.384	402.84
65.916	262.13	57.913	262.04	59.509	262.04	60.962	262.03	53.287	325.30
60.902	217.54	52.960	217.44	54.535	217.43	55.954	217.43	47.378	262.03
55.442	176.26	47.579	176.15	49.119	176.15	50.511	176.15	42.477	217.43
51.373	149.76	43.549	149.67	45.068	149.66	46.423	149.66	37.162	176.14
46.987	124.95	39.219	124.84	40.713	124.84	42.045	124.84	33.186	149.66
42.680	104.00	34.956	103.90	36.428	103.89	37.734	103.89	28.915	124.83
38.901	88.06	31.235	87.97	32.684	87.97	33.971	87.97	24.708	103.89
36.105	77.65	28.469	77.55	29.911	77.55	31.179	77.55	21.032	87.97
33.108	67.60	25.518	67.51	26.932	67.50	28.182	67.50	18.312	77.54
29.813	57.88	22.260	57.77	23.662	57.77	24.900	57.76	15.395	67.50
26.039	48.19	18.528	48.08	19.915	48.08	21.126	48.07	12.188	57.76
2,3-Dimethylpentane		2,4-Dimethylpentane		3,3-Dimethylpentane		2,2,3-Trimethylbutane		*n*-Nonane	
90.678	780.12	81.374	780.12	86.962	780.12	81.772	780.07	151.786	780.11
90.167	768.58	80.874	768.58	86.447	768.57	81.262	768.54	151.222	768.57
89.588	755.60	80.308	755.60	85.866	755.60	80.682	755.50	150.579	755.57
89.080	744.39	79.813	744.39	85.355	744.38	80.174	744.32	150.017	744.37
88.531	732.46	79.277	732.46	84.803	732.45	79.627	732.41	149.409	732.45
83.429	628.23	74.297	628.23	79.672	628.23	74.523	628.17	143.751	628.22
76.209	501.07	67.251	501.07	72.411	501.06	67.308	501.01	135.741	501.05
69.562	402.83	60.764	402.83	65.727	402.83	60.668	402.77	128.357	402.81
63.333	325.30	54.688	325.30	59.466	325.30	54.445	325.22	121.433	325.27
57.295	262.03	48.801	262.03	53.396	262.02	48.422	261.95	114.712	262.00
52.290	217.42	43.919	217.42	48.365	217.42	43.424	217.34	109.136	217.40

TABLE 1. *Experimental data for 60 hydrocarbons on the temperatures and pressures of the liquid-vapor equilibrium*—Con.

t	*P*	*t*	*P*	*t*	*P*	*t*	*P*	*t*	*P*
2,3-Dimethylpentane		2,4-Dimethylpentane		3,3-Dimethylpentane		2,3,3-Trimethylbutane		*n*-Nonane	
° *C*	*mm* Hg	° *C*	*mm* Hg	° *C*	*mm* Hg	° *C*	*mm* Hg	° *C*	*mm* Hg
46.849	176.14	38.623	176.14	42.904	176.14	38.012	176.06	103.072	176.11
42.786	149.65	34.661	149.65	38.824	149.65	33.960	149.58	98.545	149.63
38.407	124.83	30.399	124.83	34.432	124.83	29.599	124.75	93.661	124.80
34.106	103.88	26.213	103.88	30.109	103.88	25.313	103.81	88.864	103.86
30.342	87.96	22.540	87.96	------	------	21.571	87.90	84.658	87.94
27.563	77.54	19.823	77.54	23.545	77.54	18.804	77.47	81.548	77.52
24.575	67.49	16.911	67.49	20.547	67.49	15.833	67.43	78.219	67.47
21.293	57.76	13.714	57.76	17.252	57.75	12.555	57.68	74.546	57.73
17.523	48.07	------	------	13.484	48.06	------	------	70.343	48.04
2,2,5-Trimethylhexane		2,4,4-Trimethylhexane		3,3-Diethylpentane		2,2,3,3-Tetramethyl-pentane		2,2,3,4-Tetramethyl-pentane	
125.050	780.12	131.636	780.11	147.194	780.10	141.295	780.16	134.021	780.14
124.497	768.58	131.070	768.57	146.606	768.57	140.713	768.61	133.446	768.60
123.868	755.57	130.429	755.57	145.942	755.56	140.051	755.65	132.798	755.62
123.324	744.37	129.869	744.37	145.356	744.36	139.471	744.43	132.227	744.41
122.731	732.45	129.260	732.45	144.725	732.44	138.844	732.49	131.611	732.48
117.225	628.22	-------	------	138.862	628.21	133.015	628.26	125.886	628.25
109.434	501.05	115.621	501.05	130.558	501.04	124.767	501.10	117.787	501.08
102.256	402.81	108.264	402.81	122.903	402.80	117.168	402.86	110.331	402.85
95.539	325.27	101.368	325.27	115.727	325.26	110.054	325.33	103.343	325.31
-------	------	-------	------	-------	------	103.154	262.06	96.574	262.04
83.624	217.39	89.149	217.39	103.002	217.38	97.450	217.46	90.965	217.43
77.756	176.11	83.123	176.10	96.737	176.10	91.242	176.17	84.871	176.15
73.381	149.62	78.631	149.62	92.048	149.62	86.602	149.68	80.311	149.66
68.655	124.80	73.786	124.79	87.000	124.79	81.609	124.86	75.418	124.84
-------	------	69.023	103.85	82.043	103.84	76.705	103.91	70.587	103.89
59.973	87.94	64.862	87.93	77.699	87.93	72.414	87.99	66.381	87.97
56.968	77.51	61.776	77.51	74.484	77.50	69.236	77.57	63.262	77.55
53.743	67.46	58.467	67.46	71.026	67.46	65.828	67.52	59.913	67.50
50.208	57.72	54.826	57.72	67.240	57.71	62.087	57.79	56.243	57.76
46.141	48.03	50.648	48.02	62.882	48.02	57.834	48.10	52.028	48.07
2,2,4,4-Tetramethyl-pentane		2,3,3,4-Tetramethyl-pentane		Ethylcyclopentane		1,1-Dimethylcyclo-pentane		cis-1,2-Dimethylcyclo-pentane	
123.267	780.16	142.571	780.10	104.382	780.00	88.736	779.99	100.446	780.00
122.709	768.61	141.987	768.57	103.855	768.50	88.227	768.49	99.922	768.49
122.072	755.65	141.326	755.56	103.264	755.60	87.647	755.59	99.329	755.60
121.510	744.43	140.746	744.36	102.739	744.39	87.137	744.40	98.806	744.40
120.906	732.49	140.120	732.44	102.173	732.40	86.585	732.40	98.244	732.40
115.289	628.27	134.294	628.20	96.910	628.21	81.470	628.20	93.005	628.21
107.342	501.10	126.053	501.04	89.453	500.98	74.228	500.99	85.589	500.99
100.031	402.86	118.461	402.80	82.588	402.71	67.558	402.72	78.755	402.71
93.183	325.33	111.345	325.26	76.143	325.17	61.312	325.17	72.358	325.17
86.549	262.06	---------	--------	69.909	261.88	---------	--------	66.155	261.88
81.052	217.45	98.732	217.38	64.739	217.36	50.257	217.36	61.012	217.36
75.085	176.17	---------	--------	59.114	176.08	44.815	176.08	55.426	176.08
70.625	149.68	87.881	149.61	54.908	149.60	40.744	149.60	51.253	149.60
65.828	124.86	82.872	124.78	50.386	124.81	36.361	124.81	46.770	124.81
61.117	103.91	77.969	103.84	45.935	103.80	32.069	103.81	42.346	103.80
56.991	87.99	73.670	87.93	42.040	87.93	28.300	87.92	38.482	87.93
53.944	77.56	70.491	77.50	39.165	77.46	25.476	77.47	35.616	77.46
50.671	67.52	67.037	67.45	36.058	67.42	22.527	67.43	32.555	67.42
47.079	57.78	63.320	57.71	32.673	57.72	19.262	57.72	29.195	57.72
42.956	48.09	59.010	48.02	28.778	48.11	15.498	48.12	25.347	48.11

TABLE 1. *Experimental data for 60 hydrocarbons on the temperatures and pressures of the liquid-vapor equilibrium*—Con.

t	P	t	P	t	P	t	P	t	P
trans-1,2-Dimethylcyclopentane		*cis*-1,3-Dimetyhlcylcopentane		*trans*-1,3-Dimethylcyclopentane		*n*-Propylcyclopentane		Isopropylcyclopentane	
°C	*mm* Hg	°C	*mm* Hg	°C	*mm* Hg	°C	*mm* Hg	°C	*mm* Hg
92.769	780.01	92.628	780.20	91.670	780.01	131.917	780.08	127.394	780.08
92.255	768.90	92.115	768.63	91.156	768.50	131.379	768.55	126.836	768.55
91.673	755.61	91.533	755.74	90.575	755.61	130.731	755.53	126.201	755.53
91.160	744.40	91.018	744.49	90.062	744.40	130.176	744.34	125.643	744.34
90.608	732.40	90.465	732.53	---------	--------	129.579	732.42	125.044	732.42
85.463	628.22	85.315	628.32	84.368	628.22	124.015	628.19	119.450	628.19
78.181	500.99	78.030	501.15	77.092	500.99	116.132	501.03	111.532	501.03
71.466	402.71	71.323	402.93	70.388	402.71	108.877	402.79	104.235	402.79
65.178	325.17	65.039	325.41	64.105	325.18	102.068	325.25	97.396	325.25
59.094	261.88	58.949	262.13	58.029	261.88	---------	--------	90.769	261.98
54.047	217.36	53.902	217.54	52.985	217.36	89.990	217.37	85.265	217.37
48.564	176.08	48.422	176.26	47.510	176.08	84.039	176.09	79.275	176.08
44.460	149.60	44.323	149.76	43.417	149.60	79.591	149.61	74.827	149.60
40.055	124.81	39.912	124.95	39.010	124.81	74.794	124.78	70.012	124.77
35.719	103.80	35.582	104.00	34.685	103.80	70.088	103.83	65.296	103.83
31.934	87.93	31.784	88.06	30.906	87.93	65.966	87.92	61.122	87.92
29.113	77.46	28.970	77.64	28.099	77.46	62.911	77.49	58.088	77.49
26.113	67.42	25.977	67.60	25.081	67.42	59.628	67.45	54.798	67.45
---------	--------	---------	--------	21.782	57.72	56.030	57.70	51.183	57.70
---------	--------	---------	--------	18.005	48.11	51.875	48.01	47.033	48.01
1-Methyl-1-ethylcyclopentane		1-Methyl-*cis*-2-ethylcyclopentane		1,1,2-Trimethylcyclopentane		1,1,3-Trimethylcyclopentane		*cis, cis, trans*-1,2,4-Trimethylcyclopentane	
122.484	780.04	129.021	780.09	114.686	780.04	105.830	780.03	117.690	780.00
121.933	768.52	128.463	768.55	114.138	768.52	105.292	768.52	117.140	768.49
121.307	755.64	127.832	755.54	113.517	755.64	104.688	755.63	116.518	755.60
120.752	744.41	127.281	744.34	112.971	744.42	104.148	744.42	115.969	744.40
120.159	732 41	126.684	732.43	112.381	732.42	103.572	732.42	115.378	732.41
114.622	628.24	121.105	628.19	106.900	628.24	98.197	628.23	109.887	628.21
106.833	501.00	113.205	501.03	99.144	501.00	90.594	501.00	102.109	500.99
99.559	402.71	105.929	402.79	91.992	402.71	83.585	402.71	94.942	402.72
92.783	325.18	99.105	325.25	85.302	325.18	77.023	325.18	88.224	325.17
86.232	261.87	92.490	261.98	-------	------	70.674	261.88	81.725	261.89
80.796	217.37	87.011	217.38	73.455	217.37	65.411	217.37	76.327	217.36
74.888	176.09	81.050	176.09	67.615	176.09	-------	------	70.477	176.08
70.476	149.61	76.582	149.61	63.251	149.61	55.423	149.61	66.100	149.60
65.724	124.81	71.792	124.78	58.562	124.82	50.828	124.82	61.380	124.82
61.049	103.80	67.070	103.84	53.962	103.81	46.308	103.81	56.756	103.81
56.967	87.94	62.935	87.93	49.920	87.94	42.361	87.94	52.704	87.93
53.937	77.46	59.862	77.50	46.937	77.46	39.432	77.46	49.701	77.47
50.691	67.41	56.539	67.45	43.728	67.41	36.299	67.41	46.426	67.43
47.137	57.71	52.975	57.71	40.224	57.72	32.881	57.72	42.972	57.72
43.056	48.10	48.846	48.02	36.207	48.10	28.944	48.11	38.907	48.12
cis, trans, cis-1,2,4-Trimethylcyclopentane		1,1-Dimethylcyclohexane		*n*-Propylcyclohexane		Isopropylcyclohexane		1,1,3-Trimethylcyclohexane	
110.229	780.01	120.520	780.05	157.756	780.09	155.602	780.14	137.636	780.06
109.690	768.50	119.959	768.52	157.166	768.55	155.009	768.59	137.058	768.55
109.082	755.60	119.327	755.65	156.494	755.53	154.334	755.63	136.401	755.52
108.541	744.41	118.768	744.42	155.904	744.34	153.747	744.41	135.824	744.34
107.962	732.41	118.168	732.42	155.269	732.42	153.109	732.47	135.203	732.42
102.571	628.22	112.575	628.24	149.347	628.19	147.177	628.25	129.411	628.18
94.940	500.99	104.658	501.00	140.965	501.03	138.782	501.08	121.220	501.02
87.906	402.72	97.361	402.70	133.245	402.79	131.051	402.85	113.678	402.78
81.310	325.18	90.497	325.18	126.004	325.24	123.806	325.32	106.606	325.23
74.929	261.89	83.925	261.87	118.982	261.97	116.782	262.04	99.762	261.96
69.641	217.36	78.447	217.37	113.165	217.37	110.953	217.44	94.080	217.35
63.892	176.08	72.496	176.09	106.842	176.08	104.612	176.16	87.915	176.07
59.599	149.60	68.047	149.61	102.111	149.60	99.887	149.67	82.305	149.59

TABLE 1. *Experimental data for 60 hydrocarbons on the temperatures and pressures of the liquid-vapor equilibrium*—Con.

t	P	t	P	t	P	t	P	t	P
cis, trans, cis-1,2,4-Trimethylcyclopentane		1,1-Dimethylcyclohexane		*n*-Propylcyclohexane		Isopropylcyclohexane		1,1,3-Trimethylcyclohexane	
° *C*	*mm* Hg	° *C*	*mm* Hg	° *C*	*mm* Hg	° *C*	*mm* Hg	° *C*	*mm* Hg
54.976	124.82	63.260	124.81	97.017	124.77	94.793	124.85	78.336	124.76
50.433	103.81	58.564	103.80	92.026	103.83	89.788	103.90	73.481	103.82
46.454	87.93	54.450	87.94	87.641	87.92	85.400	87.98	69.180	87.91
43.487	77.47	51.399	77.46	84.375	77.49	82.165	77.56	66.058	77.48
40.338	67.43	48.153	67.40	80.871	67.44	78.690	67.51	62.624	67.43
36.878	57.72	44.531	57.71	77.085	57.70	74.868	57.78	58.950	57.68
32.948	48.11	40.497	48.10	72.691	48.01	70.515	48.09	54.669	47.99
n-Butylcyclohexane		Isobutylcyclohexane		*sec*-Butylcyclohexane		*tert*-Butylcyclohexane		Benzene	
182.024	780.09	172.394	780.16	180.421	780.15	172.670	780.10	80.948	780.04
181.406	768.56	171.780	768.60	179.799	768.60	172.054	768.56	80.461	768.51
180.706	755.53	171.089	755.65	179.098	755.64	171.351	755.54	79.909	755.48
180.093	744.34	170.480	744.43	178.481	744.42	170.735	744.35	79.424	744.29
179.433	732.43	169.822	732.49	177.817	732.48	170.071	732.43	78.903	732.38
173.272	628.19	163.711	628.26	171.626	628.26	163.894	628.20	74.035	628.15
164.544	501.03	155.065	501.09	162.856	501.09	155.147	501.03	67.148	501.00
156.504	402.79	147.103	402.86	154.776	402.86	147.093	402.79	60.803	402.76
145.963	325.24	139.640	325.33	147.212	325.32	139.542	325.25	54.852	325.21
141.651	261.97	132.404	262.05	139.861	262.05	132.228	261.98	49.084	261.95
135.579	217.36	126.405	217.45	133.786	217.45	126.159	217.37	44.294	217.34
128.988	176.08	119.887	176.17	127.163	176.16	119.573	176.08	39.095	176.06
124.056	149.60	115.008	149.68	122.224	149.67	114.649	149.60	35.207	149.58
118.743	124.77	109.766	124.86	116.900	124.85	109.341	124.77	31.013	124.75
113.535	103.82	140.610	103.91	111.660	103.90	104.146	103.83	26.908	103.81
108.963	87.91	100.094	87.98	107.082	87.98	99.582	87.92	23.271	87.90
105.579	77.48	96.767	77.56	103.688	77.56	96.200	77.49	20.628	77.47
101.946	67.44	93.184	67.51	100.048	67.51	92.550	67.44	17.697	67.42
97.950	57.69	89.248	57.78	96.042	57.78	88.600	57.70	14.575	57.68
93.369	48.00	84.752	48.09	91.458	48.09	84.033	48.00	10.983	47.98
Methylbenzene		Ethylbenzene		1,2-Dimethylbenzene		1,3-Dimethylbenzene		1,4-Dimethylbenzene	
111.545	780.05	137.160	780.06	145.400	780.07	140.078	780.07	139.329	780.06
111.018	768.52	136.602	768.53	144.832	678.54	139.520	768.54	138.768	768.53
110.420	755.49	135.969	755.50	144.190	655.52	138.887	755.51	138.132	755.51
109.894	744.30	135.413	744.32	143.626	744.33	138.329	744.32	137.574	744.32
109.328	732.39	134.815	732.40	143.019	732.41	137.731	732.41	-------	------
104.052	628.16	129.234	628.17	137.356	628.18	132.144	628.17	131.371	628.17
96.580	501.00	121.331	501.01	129.333	501.02	124.226	501.01	123.431	501.01
89.695	402.76	114.046	402.77	121.935	402.78	116.923	402.78	-------	------
83.230	325.22	107.210	325.23	114.988	325.24	110.067	325.23	109.240	325.22
76.965	261.95	100.576	261.96	108.250	261.97	103.412	261.96	102.573	261.96
71.758	217.34	95.074	217.35	102.657	217.36	97.887	217.36	97.032	217.35
66.107	176.06	89.090	176.07	96.568	176.08	91.874	176.07	91.017	176.07
61.869	149.58	84.619	149.59	92.015	149.60	87.387	149.60	86.506	149.59
57.315	124.75	79.791	124.76	87.101	124.77	81.527	124.76	81.658	124.76
52.848	103.81	75.054	103.81	82.285	103.83	77.778	103.82	76.885	103.82
48.894	87.90	70.891	87.91	78.048	87.92	73.601	87.91	72.684	87.91
45.997	77.47	67.827	77.48	74.916	77.49	70.506	77.48	69.605	77.48
-------	------	64.510	67.43	71.548	67.44	67.157	67.44	66.280	67.43
39.437	57.68	60.887	57.68	67.852	57.70	63.518	57.69	62.619	57.68
35.504	47.99	56.689	47.99	63.608	48.01	59.335	48.00	58.419	47.99
n-Propylbenzene		Isopropylbenzene		1-Methyl-2-ethylbenzene		1-Methyl-3-ethylbenzene		1-Methyl-4-ethylbenzene	
160.239	780.09	153.40	780.09	166.174	779.94	162.316	779.94	163.008	779.95
159.654	768.55	152.82	768.55	165.591	768.46	161.735	768.46	162.424	768.46
158.991	755.54	152.17	755.54	164.925	755.53	161.080	755.54	161.761	755.55
158.408	744.35	151.59	744.34	164.337	744.38	160.498	744.38	161.179	744.39
157.779	732.43	150.97	732.43	163.706	732.39	159.871	732.39	160.548	732.39

TABLE 1. *Experimental data for 60 hydrocarbons on the temperatures and pressures of the liquid-vapor equilibrium*—Con.

t	P	t	P	t	P	t	P	t	P
n-Propylbenzene		Isopropylbenzene		1-Methyl-2-ethylbenzene		1-Methyl-3-ethylbenzene		1-Methyl-4-ethylbenzene	
° *C*	*mm* Hg	° *C*	*mm* Hg	° *C*	*mm* Hg	° *C*	*mm* Hg	° *C*	*mm* Hg
151.921	628.20	145.19	628.19	157.825	628.17	154.053	628.17	154.684	628.18
143.625	501.03	137.01	501.03	149.482	500.98	145.795	500.98	146.368	500.98
135.972	402.80	129.46	402.79	141.792	402.73	138.178	402.73	138.701	402.73
128.794	325.26	122.38	325.25	134.570	325.16	131.027	325.16	131.499	325.16
---	---	115.52	261.98	127.574	261.92	124.082	261.92	---	---
116.060	217.38	109.82	217.37	121.762	217.35	118.338	217.35	118.727	217.35
109.781	176.09	103.64	176.09	115.436	176.06	112.074	176.06	112.422	176.07
105.085	149.61	99.00	149.61	110.711	149.59	107.383	149.59	107.710	149.59
100.020	124.78	94.01	124.78	105.598	124.82	102.326	124.82	102.619	124.82
95.049	103.84	89.11	103.83	100.584	103.81	97.368	103.81	97.630	103.81
90.688	87.93	84.82	87.92	96.200	87.91	93.022	87.91	93.252	87.91
87.457	77.50	81.64	77.49	92.949	77.43	89.793	77.47	89.988	77.47
83.993	67.45	78.23	67.45	89.448	67.45	86.293	67.45	86.523	67.45
80.181	57.71	74.47	57.70	85.618	57.73	82.525	57.73	82.701	57.43
75.818	48.02	70.16	48.01	81.146	48.13	78.105	48.13	78.306	48.13
1,2,3-Trimethylbenzene		1,2,4-Trimethylbenzene		1,3,5-Trimethylbenzene		*n*-Butylbenzene		Isobutylbenzene	
177.126	779.95	170.377	779.96	165.725	779.97	184.329	779.98	173.814	779.99
176.527	768.46	169.788	768.47	165.146	768.47	183.725	768.48	173.209	768.49
175.852	755.55	169.121	755.55	164.489	755.56	183.036	755.57	172.526	755.59
175.252	744.34	168.534	744.39	163.911	744.39	182.429	744.40	171.920	744.41
174.606	732.39	167.896	732.39	163.289	732.39	181.767	732.40	171.270	732.41
168.614	628.18	161.991	628.18	157.477	628.19	175.666	628.20	165.217	628.21
160.106	500.98	153.603	500.98	149.228	500.98	167.011	500.99	156.632	500.99
152.260	402.72	145.867	402.72	141.618	402.72	159.032	402.73	148.724	402.73
144.882	325.16	138.599	325.16	134.464	325.17	151.541	325.17	141.301	325.17
137.737	261.91	131.556	261.91	---	---	-- ------	-------	134.112	261.91
131.800	217.35	125.694	217.35	121.765	217.36	138.300	217.36	128.149	217.36
125.333	176.07	119.328	176.07	115.489	176.07	---	---	121.659	176.07
120.504	149.59	114.572	149.59	110.789	149.59	126.797	149.60	116.808	149.60
115.287	124.81	109.418	124.81	105.716	124.82	121.506	124.82	111.582	124.82
110.157	103.81	104.369	103.81	100.747	103.81	116.322	103.81	106.450	103.81
105.663	87.91	99.940	87.91	96.386	87.92	111.762	87.92	101.946	87.92
102.336	77.47	96.650	77.47	93.131	77.47	108.403	77.47	98.620	77.47
98.770	67.45	93.155	67.44	89.662	67.44	104.778	67.44	95.026	67.44
94.826	57.73	89.259	57.73	85.857	57.73	100.814	57.73	91.118	57.73
90.332	48.13	84.804	48.13	81.488	48.12	96.233	48.12	86.637	48.12
sec-Butylbenzene		*tert*-Butylbenzene		1,2-Diethylbenzene		1,3-Diethylbenzene		1,4-Diethylbenzene	
174.358	779.99	170.165	780.00	184.493	780.21	182.162	780.20	184.821	780.20
173.754	768.49	169.565	768.50	183.885	768.64	181.558	768.64	184.212	768.63
173.068	755.59	168.886	755.59	183.197	755.75	180.877	755.74	183.524	755.73
172.468	744.40	168.287	744.41	182.590	744.50	180.275	744.49	182.916	744.49
171.820	732.41	167.646	732.41	181.936	732.54	179.628	732.53	182.260	732.53
165.768	628.21	161.649	628.21	175.853	628.32	173.595	628.31	176.164	628.31
157.194	500.99	153.149	500.99	167.235	501.16	165.050	501.15	167.530	501.14
149.288	402.73	145.315	402.72	159.290	402.93	157.169	402.92	159.566	402.92
141.867	325.17	137.968	325.18	151.832	325.42	149.777	325.41	152.086	325.40
134.683	261.90	---	---	144.596	262.13	142.597	262.12	144.823	262.12
128.715	217.36	124.936	217.36	138.590	217.54	136.638	217.53	138.811	217.53
122.232	176.08	118.524	176.08	132.059	176.26	130.157	176.25	132.256	176.24
117.387	149.60	113.720	149.60	127.171	149.76	125.303	149.75	127.360	149.75
112.151	124.82	108.546	124.82	121.906	124.95	120.082	124.94	122.043	124.94
107.009	103.81	103.471	103.81	116.728	104.00	114.946	103.98	116.893	103.98
102.523	87.92	99.017	87.92	112.191	88.05	110.436	88.04	112.339	88.04
99.179	77.47	95.715	77.50	108.822	77.64	107.096	77.63	108.962	77.63
95.620	67.43	92.194	67.43	105.223	67.59	103.524	67.58	105.353	67.58
91,684	57.72	88.312	57.72	101.263	57.88	99.573	57.86	101.370	57.86
87.118	48.12	83.877	48.20	96.729	48.19	95.092	48.18	96.817	48.17

VI. Correlation of the Data With the Antoine Equation

The method of correlation has been described previously [1]. The values of the three constants of the Antoine equation for vapor pressures, obtained from the data in table 1, are given in table 2, together with the ranges of pressure and temperature over which the experimental data were obtained (and over which, therefore, the resulting equation for each compound is applicable without loss of accuracy). The values of the boiling point and the pressure coefficient of the boiling point at 760.00 mm Hg, calculated from the Antoine equation, are also given.

The last column of table 2 gives, for each compound, the root-mean-square value, ρ, of the ratios of the deviations of the observed points from the Antoine equation to the expected standard deviations. The expected deviations were calculated on the basis of standard deviations (of a single value) of ± 0.003 deg C in the temperature and ± 0.06 to ± 0.11 mm Hg in the pressure, for the lowest and highest pressures, respectively. The values of ρ for the 60 compounds vary from 0.24 to 1.75, whereas the over-all value of ρ, computed for the total of 1,169 points on 60 compounds, is 0.56.

TABLE 2. *Summary of the results of the correlation of the experimental data with the Antoine equation for vapor pressures, for 60 API-NBS hydrocarbons*

Compound	Formula	Constants of the Antoine equation $\log_{10} P = A - B/(C+t)$, or $t = B/(A - \log_{10} P) - C$ (P in mm Hg; t in ° C)			Normal boiling point at 760 mm Hg	Pressure coefficient, dt/dP, at 760 mm Hg	Range of measurement		Measure of precisions
		A	B	C			Pressure	Temperature	ρ
PARAFFINS									
					° C	° C/mm Hg	mm Hg	° C	
n-Heptane	C_7H_{16}	6.90027	1266.871	216.757	98.427	0.04481	48 to 780	26.0 to 99.3	0.36
2-Methylhexane	C_7H_{16}	6.87319	1236.026	219.545	90.052	.04431	48 to 780	18.5 to 90.9	.43
3-Methylhexane	C_7H_{16}	6.86764	1240.196	219.223	91.850	.04459	48 to 780	19.9 to 92.7	.38
3-Ethylpentane	C_7H_{16}	6.87565	1251.827	219.887	93.475	.04482	48 to 780	21.1 to 94.4	.61
2,2-Dimethylpentane	C_7H_{16}	6.81479	1190.033	223.303	79.197	.04394	58 to 780	12.2 to 80.1	.29
2,3-Dimethylpentane	C_7H_{16}	6.85382	1238.017	221.823	89.784	.04482	48 to 780	17.5 to 90.7	.33
2,4-Dimethylpentane	C_7H_{16}	6.82621	1192.041	221.634	80.500	.04376	58 to 780	13.7 to 81.4	.40
3,3-Dimethylpentane	C_7H_{16}	6.82668	1228.663	225.316	86.064	.04509	48 to 780	13.5 to 87.0	.28
2,2,3-Trimethylbutane	C_7H_{16}	6.79230	1200.563	226.050	80.882	.04484	58 to 780	12.6 to 81.8	.33
n-Nonane	C_9H_{20}	6.93513	1428.811	201.619	150.798	.04967	48 to 780	70.3 to 151.8	.24
2,2,5-Trimethylhexane	C_9H_{20}	6.83532	1324.049	210.737	124.084	.04838	48 to 780	46.1 to 125.0	.39
2,4,4-Trimethylhexane	C_9H_{20}	6.85164	1368.723	214.047	130.648	.04960	48 to 780	50.6 to 131.6	.55
3,3-Diethylpentane	C_9H_{20}	6.89262	1451.245	215.575	146.168	.05109	48 to 780	62.9 to 147.2	.43
2,2,3,3-Tetramethylpentane	C_9H_{20}	6.82876	1397.483	213.703	140.274	.05124	48 to 780	57.8 to 141.3	.36
2,2,3,4-Tetramethylpentane	C_9H_{20}	6.83173	1374.042	214.762	133.016	.05030	48 to 780	52.0 to 134.0	.43
2,2,4,4-Tetramethylpentane	C_9H_{20}	6.79711	1325.183	216.093	122.284	.04937	48 to 780	43.0 to 123.3	.37
2,3,3,4-Tetramethylpentane	C_9H_{20}	6.85961	1417.473	214.705	141.551	.04223	48 to 780	59.0 to 142.6	.49
ALKYLCYCLOPENTANES									
Ethylcyclopentane	C_7H_{14}	6.88709	1298.599	220.675	103.466	0.04623	48 to 780	28.8 to 104.4	0.52
1,1-Dimethylcyclopentane	C_7H_{14}	6.81725	1219.474	221.946	87.846	.04497	48 to 780	15.5 to 88.7	.59
cis-1,2-Dimethylcyclopentane	C_7H_{14}	6.85008	1269.140	220.209	99.532	.04603	48 to 780	25.3 to 100.4	.39
trans-1,2-Dimethylcyclopentane	C_7H_{14}	6.84422	1242.748	221.686	91.869	.04521	67 to 780	26.1 to 92.8	.75
cis-1,3-Dimethylcyclopentane	C_7H_{14}	6.83817	1240.023	221.621	91.725	.04525	67 to 780	26.0 to 92.6	.30
trans-1,3-Dimethylcyclopentane	C_7H_{14}	6.83715	1237.456	222.005	90.773	.04518	48 to 780	18.0 to 91.7	.51
n-Propylcyclopentane	C_8H_{16}	6.90392	1384.386	213.159	130.949	.04888	48 to 780	51.9 to 131.9	.74
Isopropylcyclopentane	C_8H_{16}	6.88623	1379.415	217.969	126.419	.04913	48 to 780	47.0 to 127.4	.55
1-Methyl-1-ethylcyclopentane	C_8H_{16}	6.87149	1355.287	218.092	121.522	.04863	48 to 780	43.1 to 122.5	1.75
1-Methyl-*cis*-2-ethylcyclopentane	C_8H_{16}	6.90562	1388.307	216.888	128.050	.04897	48 to 780	48.8 to 129.0	0.25
1,1,2-Trimethylcyclopentane	C_8H_{16}	6.82206	1309.618	218.557	113.729	.04818	48 to 780	36.2 to 114.7	.46
1,1,3-Trimethylcyclopentane	C_8H_{16}	6.80948	1275.998	219.899	104.893	.04724	48 to 780	28.9 to 105.8	.40
cis-cis-trans-1,2,4-Trimethylcyclopentane	C_8H_{16}	6.85448	1333.894	218.952	116.731	.04827	48 to 780	38.9 to 117.7	.71
cis, trans, cis-1,2,4-Trimethylcyclopentane	C_8H_{16}	6.84971	1306.153	219.808	109.290	.04738	48 to 780	32.9 to 110.2	.38

TABLE 2. *Summary of the results of the correlation of the experimental data with the Antoine equation for vapor pressures, for 60 API-NBS hydrocarbons*—Continued

Compound	Formula	Constants of the Antoine equation $\log_{10} P=A-B/(C+t)$, or $t=P/(A-\log_{10} P)-C$ (P in mm Hg; t in ° C)			Normal boiling point at 760 mm Hg	Pressure coefficient, dt/dP, at 760 mm Hg	Range of measurement		Measure of precision
		A	B	C			Pressure	Temperature	ρ
ALKYLCYCLOHEXANES									
					° C	° C/mm Hg	mm Hg	° C	
1,1-Dimethylcyclohexane	C_8H_{16}	6.80225	1323.861	218.053	119.543	0.04920	48 to 780	40.5 to 120.5	1.25
n-Propylcyclohexane	C_9H_{18}	6.88866	1461.715	207.990	156.724	.05200	48 to 780	72.7 to 157.8	0.59
Isopropylcyclohexane	C_9H_{18}	6.87257	1452.816	209.391	154.563	.05210	48 to 780	70.5 to 155.6	.30
1,1,3-Trimethylcyclohexane	C_9H_{18}	6.83705	1393.299	215.551	136.626	.05089	48 to 780	54.7 to 137.6	.60
n-Butylcyclohexane	$C_{10}H_{20}$	6.91261	1539.449	200.880	180.947	.05412	48 to 780	93.4 to 182.0	.30
Isobutylcyclohexane	$C_{10}H_{20}$	6.86703	1492.462	203.085	171.321	.05367	48 to 780	84.8 to 172.4	.32
sec-Butylcyclohexane	$C_{10}H_{20}$	6.88907	1529.373	202.220	179.335	.05440	48 to 780	91.4 to 180.4	.59
tert-Butylcyclohexane	$C_{10}H_{20}$	6.85449	1500.118	205.923	171.591	.05429	48 to 780	84.0 to 172.7	.45
ALKYLBENZENES									
Benzene	C_6H_6	6.91210	1214.645	221.205	80.099	0.04271	48 to 780	10.9 to 80.9	0.82
Methylbenzene	C_7H_8	6.95508	1345.087	219.516	110.626	.04630	48 to 780	35.5 to 111.5	.54
Ethylbenzene	C_8H_{10}	6.95904	1425.464	213.345	136.186	.04898	48 to 780	56.7 to 137.2	.56
1,2-Dimethylbenzene	C_8H_{10}	6.99891	1474.679	213.686	144.411	.04969	48 to 780	63.6 to 145.4	.43
1,3-Dimethylbenzene	C_8H_{10}	7.00849	1461.925	215.073	139.104	.04903	48 to 780	59.3 to 140.1	.40
1,4-Dimethylbenzene	C_8H_{10}	6.99184	1454.328	215.411	138.351	.04917	48 to 780	58.4 to 139.3	.46
n-Propylbenzene	C_9H_{12}	6.95094	1490.963	207.100	159.218	.05143	48 to 780	75.8 to 160.2	.43
Isopropylbenzene	C_9H_{12}	6.93958	1462.717	207.993	152.392	.05074	48 to 780	70.2 to 153.4	.39
1-Methyl-2-ethylbenzene	C_9H_{12}	7.00314	1535.374	207.300	165.153	.05163	48 to 780	81.1 to 166.2	1.18
1-Methyl-3-ethylbenzene	C_9H_{12}	7.01582	1529.184	208.509	161.305	.05111	48 to 780	78.1 to 162.3	1.12
1-Methyl-4-ethylbenzene	C_9H_{12}	6.99801	1527.113	208.921	161.989	.05148	48 to 780	78.3 to 163.0	0.68
1,2,3-Trimethylbenzene	C_9H_{12}	7.04082	1593.958	207.078	176.084	.05263	48 to 780	90.3 to 177.1	.66
1,2,4-Trimethylbenzene	C_9H_{12}	7.04383	1573.267	208.564	169.351	.05187	48 to 780	84.8 to 170.4	.83
1,3,5-Trimethylbenzene	C_9H_{12}	7.07437	1569.622	209.578	164.716	.05100	48 to 780	81.5 to 165.7	.53
n-Butylbenzene	$C_{10}H_{14}$	6.98318	1577.965	201.378	183.270	.05358	48 to 780	96.2 to 184.3	1.38
Isobutylbenzene	$C_{10}H_{14}$	6.93033	1526.384	204.171	172.759	.05319	48 to 780	86.6 to 173.8	0.34
sec-Butylbenzene	$C_{10}H_{14}$	6.95097	1540.174	205.101	173.305	.05313	48 to 780	87.1 to 174.4	1.03
tert-Butylbenzene	$C_{10}H_{14}$	6.92050	1504.572	203.328	169.119	.05269	48 to 780	83.9 to 170.2	0.73
1,2-Diethylbenzene	$C_{10}H_{14}$	6.99016	1577.894	200.554	183.423	.05340	48 to 780	96.7 to 184.5	.43
1,3-Diethylbenzene	$C_{10}H_{14}$	7.00601	1576.261	201.004	181.102	.05293	48 to 780	95.1 to 182.2	.49
1,4-Diethylbenzene	$C_{10}H_{14}$	7.00054	1589.273	202.019	183.752	.05351	48 to 780	96.8 to 184.8	.62

VII. Discussion

The vapor pressures of different samples of 15 of the above hydrocarbons have been previously measured in this laboratory [1]. Table 3 gives, for each of these 15 hydrocarbons, the calculated difference in pressure for a low, intermediate, and high temperature and the calculated difference in temperature for a low (50 mm Hg), intermediate (250 mm Hg), and high (760 mm Hg) pressure, in the range of measurement. Omitting two compounds, *n*-propylcyclopentane and *n*-propylcyclohexane, of which the previous samples contained a significantly greater amount of impurity, the average differences in temperature and in pressure at each of the three levels are seen to be quite satisfactory.

TABLE 3. *Comparison of the data obtained on 15 compounds in this and the previous investigation [1]*

Compound	Temperature	Calculated difference in pressure	Pressure	Calculated difference in temperature
	°C	*mm Hg*	*mm Hg*	°C
n-Heptane	98.427	−0.05	760	0.002
	64.624	.01	250	−.001
	26.811	−.01	50	.002
2,2-Dimethylpentane	79.197	.10	760	−.005
	46.127	.02	250	−.002
	9.315	−.01	50	.002
3,3-Dimethylpentane	86.064	.11	760	−.004
	52.113	.07	250	−.008
	14.296	.07	50	−.029
n-Nonane	150.798	−.04	760	.002
	113.292	.03	250	−.004
	71.255	−.02	50	.013
n-Propylcyclopentane	130.949	−.26	760	.012
	94.074	.05	250	−.006
	52.816	.09	50	−.039
Isopropylcyclopentane	126.419	−.08	760	.005
	89.367	.04	250	−.006
	47.955	.06	50	−.028
n-Propylcyclohexane	156.724	−.24	760	.013
	117.507	−.08	250	.010
	73.667	.02	50	−.007
Benzene	80.099	.07	760	−.003
	47.869	.05	250	−.006
	11.792	.11	50	−.046
Methylbenzene	110.626	−.07	760	.003
	75.644	−.01	250	.001
	36.393	.01	50	−.005
Ethylbenzene	136.186	.02	760	.000
	99.181	.02	250	−.006
	57.652	.07	50	−.031
1,2-Dimethylbenzene	144.411	.05	760	−.002
	106.828	.02	250	−.004
	64.558	.01	50	−.003
1,3-Dimethylbenzene	139.104	−.03	760	.002
	102.010	.06	250	−.006
	60.267	.06	50	−.027
1,4-Dimethylbenzene	138.351	−.08	760	.003
	101.167	−.02	250	.002
	59.360	.03	50	−.011
n-Propylbenzene	159.218	−.06	760	.003
	120.368	−.03	250	.003
	76.786	.00	50	.005
Isopropylbenzene	152.392	.02	760	.000
	114.075	−.01	250	.002
	71.119	.04	50	−.020

Average	For temperature corresponding to—	Calculated difference in pressure	at—	Calculated difference in temperature
Average	760 mm	0.060	760 mm	0.0026
	250 mm	.030	250 mm	.0039
	50 mm	.038	50 mm	.0171

In the previous report [1], it was pointed out that some correlation exists between the values of the constants B and C of the Antoine equation and the number of carbon atoms in the normal alkyl side chain for the members of several normal alkyl series of hydrocarbons, as normal paraffins, normal alkylcyclopentanes, normal alkylcyclohexanes, and normal alkylbenzenes. For the previous correlation, values for ethylcyclopentane, *n*-butylcyclohexane, and *n*-butylbenzene were not available. The values of the B and C constants for these three compounds obtained from the present investigation are found to be in good accord with those previously reported for the neighboring members of these series [1].

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